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Two-Spin-Majority Cellular Automaton as a Model of 2D Cluster and Interface Growth

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A new probabilistic cellular automaton model is introduced to simulate cluster and interface growth in two dimensions. The dynamics of this model is an extension to higher dimensions of the compact directed percolation studied by Essam. Numerical results indicate that the two-dimensional cluster coarsening and growth can be described only approximately by the conventional cluster size scaling due to a crossover in the growth mode. The spreading of the initially flat interface follows a purely diffusional, $t^{1/2}$, law.

KEY WORDS: Cluster size scaling; cellular automata; interfacial dynamics; phase separation.

Studies of cluster properties and, specifically, the cluster size distribution in aggregation models[1] and at phase separation, e.g., spinodal decomposition,[2,3] usually involve complicated systems and require substantial numerical resources. It is therefore of interest to develop simplied lattice cellular automata-type models which show effects reminiscent of phase separation and cluster coarsening. The price paid is that usually such models do not have detailed balance dynamics. One such simplified model is introduced in this note; we report various numerical results on the cluster size distribution and on certain interfacial properties.

The idea of mimicking spinodal decomposition by a cellular automaton-type generalized *voter model* was introduced by Scheucher and Spohn.[4] The dynamics of their model is given by the rule that a spin ± 1 on a hypercubic lattice flips at the rate $\lambda n/2D$, $n = 0, 1, 2, \ldots, 2D$, where $n/2D$

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is the fraction of its neighbors pointing in the opposite direction, while λ sets the time scale. Scheucher and Spohn[4] presented results of numerical simulations for the cluster size distribution in two dimensions. They found that after a short time the cluster size distribution follows an effective power law behavior. They further commented that, although the apparent exponent τ values (see below) vary somewhat with time, there is no systematic time dependence.

For varying dimensionality D, the voter model[4] shows "phase separation"-type behavior (i.e., the coarsening of the $\pm$-spin clusters) only in $D=1, 2$, but not for higher dimensions, $D=3, 4,\ldots$. This property was argued for[4] based on the fact that the dynamics of the model relates to the statistics of two random walks meeting.

In this note we introduce the two-spin-majority automaton model which has the following new useful features: (a) the dynamics is easy to simulate numerically and it generalizes in an obvious way from $D=1$ to $D=2$ and to higher D values; (b) the model involves a parameter p which can be varied to break the ± 1 spin symmetry, thus favoring the $+$ phase for $p>1/2$ and the $-$ phase for $p<1/2$; see below. This model is an extension to $(D+\text{time})>2$ of the $(1+\text{time})$-dimensional directed compact percolation.[5] We emphasize the $(D=2)$-dimensional cluster and interface growth aspects in this note. A study of exponents in the $(D+\text{time})$ directed percolation nomenclature would be of interest, but it is not attempted here.

Let us consider first the one-dimensional case. If the time axis is plotted perpendicular to the direction of the one-dimensional space axis, then we define the $(1+1)$-dimensional "connectivity" to have the resulting square lattice with the axes rotated 45° with respect to the space and time directions. The particular automaton rule is as follows: if two adjacent spins are both $+1$ (both -1) at time t, then at time $(t+1)$ there will be spin $+1$ (-1) at the interstice between them. If one spin has the value $+1$, the other the value -1, then the new spin is chosen to have the value $+1$ with probability p, and -1 otherwise (probability $1-p$). The model was originally formulated[5] as a compact-cluster directed percolation in $(1+1)$ dimensions. In the one-dimensional nomenclature, the interstices form the same lattice as the original one, shifted by half the lattice spacing.

The kinetics of the model in the one-dimensional case is characterized by the dynamics of the domain walls separating $+$ and $-$ regions. Indeed, the domain wall motion is diffusional for $p=1/2$, and pairs of walls annihilate in each encounter, thus leading to cluster growth. While there are no exact results for the cluster size distribution for this model, numerous numerical, exact, and asymptotic results were obtained[5–10] for several diffusive-domain-wall models in one dimension, for many interesting properties. These results will not be reviewed here. (Cluster size

exponent values in one dimension will be quoted below.) For $p > 1/2$ and $p < 1/2$ the domain wall motion is that of diffusion with the superimposed drift that favors growth of the + clusters or − clusters, respectively. The model is obviously self-dual with respect to $(+ \leftrightarrow -)$ accompanied by $(p \leftrightarrow 1-p)$.

In higher dimensions, in a given time step one considers all pairs of sites in one particular lattice direction and updates the spins according to the one-dimensional rule. The resulting spins in the interstices form the same hypercubic lattice, shifted by half the lattice spacing. One then proceeds in the same way with pairs along the second dimension, and so on. Thus, the full round of updating takes D time steps. In those time steps the updating rule is applied consecutively along the D lattice axes.

For $p > 1/2$, the system evolves from any randomly populated initial configuration toward an equilibrium state consisting of +1's everywhere. Even though the probability p can take on values in [0, 1], in practice our simulations show that the approach to the + state is very rapid unless p is quite close to 1/2. Convenient p values to observe a growth of a + cluster from a small seed cluster in the background of − spins are about $p \simeq 0.51$ or somewhat greater.

The self-dual system at $p = 1/2$ corresponds to a kinetic first-order transition. As mentioned, the present model has no equilibrium states and detailed balance is not satisfied. The states $\pm$ are "absorbing" from the point of view of the stochastic dynamics, and they are equally probable at $p = 1/2$ (for general initial conditions). The coarsening of the $\pm$ clusters at $p = 1/2$ was studied numerically in two dimensions; see below. As for the voter model,[4] the behavior in higher dimensions may differ from that in two dimensions. The present study was restricted to $D = 2$.

Detailed structural information is provided by the cluster size distribution. We start with a random configuration of spins on a 200×200 square lattice with helical boundary conditions along one direction and periodic boundary conditions along the other. The number of the s-site clusters (both + and −), normalized per lattice site, $n_s(t)$, is determined by the Hoshen–Kopelman[11] method. Cluster sizes s are grouped for statistical purposes, with a separate bin for each doubling in size, i.e., a bin corresponds to cluster sizes 2^b to $(2^{b+1} - 1)$, $b = 0, 1, 2, \ldots$. The arithmetic mean value of a bin's range is denoted by $\bar{s}$. Thus, the bins cover sizes 1 to 1, 2 to 3, 4 to 7, etc., so that $\bar{s}$ is 1, 2.5, 5.5, respectively. Note that for studying power law cluster size behavior (see below) one can use the geometrical mean value for each bin or several other size measures; the results are not sensitive to a particular choice. The cumulative cluster numbers for each bin will be denoted $n_{\bar{s}}$. The results for 4, 16, 64, and 256 Monte Carlo (MC) steps are presented in Fig. 1. Each Monte Carlo step

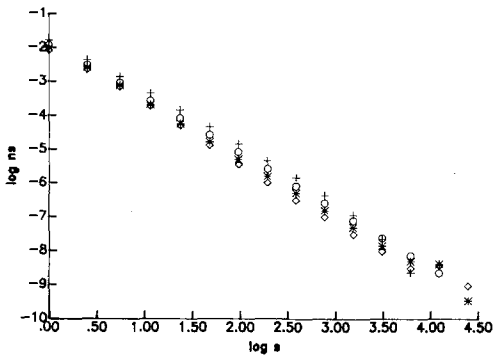

Fig. 1. Cluster size distribution $n_s(t)$ vs. s for the two-spin-majority model on a 200×200 square lattice for $t = 4$ MCs (+), 16 MCs (○), 64 MCs (∗), and 256 MCs (◇).

(MCs) here means a full update along $D = 2$ directions, i.e., two original unit-time steps according to the definition of the model. (The computations reported in this communication took several CPU hours on the Cray-YMP supercomputer at HLRZ.)

The cluster size distribution seemingly develops quickly toward a power law behavior

$$n_s \simeq a(t)\, s^{-\tau} \tag{1}$$

However, closer examination reveals that the exponent τ may not be well-defined in two dimensions; see below. For growth models one usually assumes the cluster size distribution scaling of the form[2,12]

$$n_s(t) \approx s^{-2} F(s/t^z) \tag{2}$$

where z is the dynamic critical exponent. For large times, i.e., for $s/t^z \ll 1$, one assumes

$$F(x \ll 1) \propto x^{2-\tau} \tag{3}$$

Note that in one dimension the exponents are $\tau = -1$ and $z = 1/2$. The cluster size scaling applies, and the scaling function $F(x)$ has been studied numerically.[10] Its large-x behavior is an exponential decay (for $D = 1$).

Generally, the scaling forms (2)–(3) are valid for $\tau < 2$ and suggest the buildup of the power law cluster size distribution (1) with $a(t) \sim t^{z(2-\tau)}$. The time dependence of the coefficient is difficult to confirm due to the smallness of the difference $(2 - \tau)$; see below. However, the power law s-dependence is clearly seen in Fig. 1.

Initially, the apparent exponent τ increases systematically with time. This can also be seen on the basis of Fig. 2, which is a plot of cluster numbers at fixed size $\bar{s}$ as a function of time up to 8192 MCs for several values of $\bar{s}$. To more clearly illustrate the differences between cluster sizes, we show the change in $n_{\bar{s}}$ from its initial value (actually, its value at $t=2$ MCs). At small times, say less than 100 or 200 MCs, $n_{\bar{s}}$ for larger clusters decreases more rapidly, causing the apparent τ value to increase.

For each cluster size there exists a crossover to a much lower rate of decrease. This crossover occurs progressively later (and is sharper) for larger clusters. What is important to note is that at this later stage the number of smaller clusters decreases more rapidly than the larger ones. This is not readily apparent from Fig. 2, but can be seen to be the case from Fig. 3, in which we collapse the data at $t=128$ MCs to the same point and plot the subsequent changes in $n_{\bar{s}}$. Clearly, the smaller clusters decrease more rapidly, which leads to a decrease in the value of τ. We see that, in fact, the exponent τ undergoes a systematic change with time and is not well-defined. After an initial period in which it increases with time to a maximum value approaching 2, there is a crossover to a decreasing τ.

In the absence of data for extremely large times, we can only conjecture a possible scenario for the breakdown of the cluster size scaling, relations (1)–(3). The most plausible one is that the growth proceeds in two stages. Initially, clusters of all sizes coarsen, and the scaling applies. In the later stage the growth mode changes: the largest clusters "eat up" the smaller clusters and dominate the growth process. A similar mechanism may be responsible for the absence of a systematic trend in the apparent τ values found for the voter model.[4]

We also studied the roughness of a growing interface between spin $+1$ and spin -1 regions. One starts with two semi-infinite regions with spins

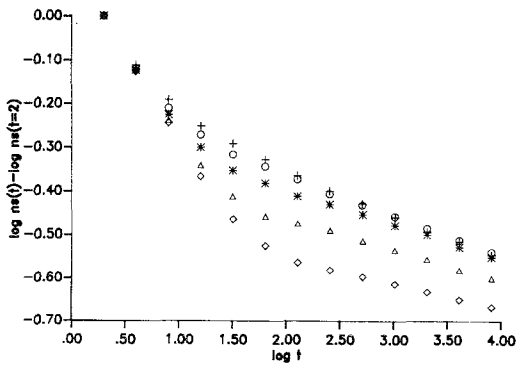

Fig. 2. Change in $n_{\bar{s}}$ with time t for $\bar{s}=1$ (+), 2.5 (○), 5.5 (*), 11.5 (△), 23.5 (◇).

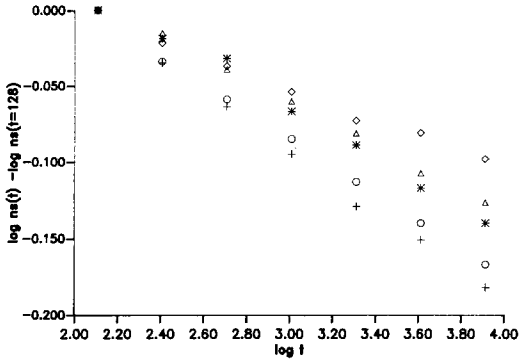

Fig. 3. Change in $n_{\bar{s}}$ with time after $t = 128$ MCs; see text. Cluster sizes are the same as for Fig. 2.

$+1$ on the left and spins -1 on the right separated by a flat vertical interface of length L. In these simulations we used $L = 300$ and periodic boundary conditions in both directions; thus, the second interface was present on the opposite side of the lattice. However, in the simulations, the "main" interface has never grown large enough to reach all the way around, so that no special consideration of the boundary-condition-related finite-size effects was needed.

Following Derrida and Dickman,[13] we define the width of the interface as

$$W(t) = \sum_i [1 - m_{i,j}^2(t)] \tag{4}$$

where $m_{i,j}(t) = \langle \sigma_{i,j}(t) \rangle$ is the average over independent realizations, of the spin at a site (i, j), with i referring to the horizontal coordinate and j to the vertical coordinate. The sum is over all sites having the same value of j. Because of periodic boundary conditions, this result is independent of j. Note that while the definition (4) is computationally convenient, it can only be used in the problems in which the profile $\langle \sigma \rangle$ converges rapidly enough to the asymptotic values at the far right (-1 in our case) and far left ($+1$). Our numerical results are presented in Fig. 4. A clear indication was found for the diffusive interface width growth,

$$W(t) \sim t^{1/2} \tag{5}$$

We are not aware of any results for other automaton models, such as the voter model, to be compared with (5). A study of surface roughening in the deterministic Q2R automata is currently in progress.[14]

In conclusion, the two-spin-majority automaton provides a convenient test model for cluster and interface growth. The most interesting result of

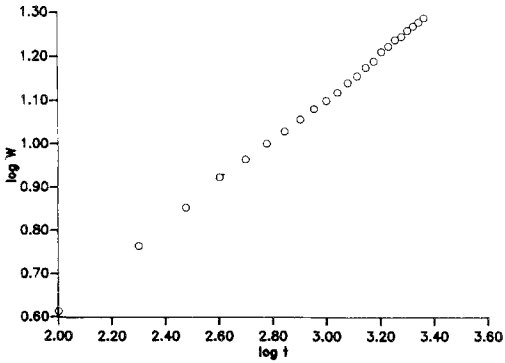

Fig. 4. Width $W(t)$ of an interface as a function of time t for system size $L = 300$.

our numerical study in two dimensions is the breakdown of the simple cluster size scaling description. To the extent that the concept of universality applies here, the two-spin model seems to be in the same universality class as the voter model.

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